

TOLUENE

In formulations where Toluene is present in relatively small amounts, Toluene can be replaced by Methyl Cyclohexane and/or acetates almost as a direct drop in as long as evaporation rates of the final blend are similar.

Examples of such possible substitutions are given in Table V.

Table V

Compound wt %	Reference	Blend 1	Blend 2
Solane 60/95	60	55	60
n-Propyl Acetate	-	-	10
Methyl cyclohexane		15	
Methyl Ethyl Ketone	30	30	30
Toluene	10	-	-
Density	0.719	0.717	0.720
Hansen Solubility Parameters (sqrt/ J/cm³)			
δ <sub>D</sub>	2.54	2.42	2.80
δ <sub>H</sub>	1.54	1.39	2.00
δ <sub>P</sub>	15.58	15.47	15.36
δ total	15.86	15.71	15.73

For adhesives applications, such as polychloroprene based adhesives, Toluene is often present in a fairly large quantity. In this case, the substitution will have to take into account additional factors such as the rheological behavior of the final blend during application. The ratio of the solvents to be used should take into account both the final solubility parameters, as these dictate the miscibility and solvency power, as well as the final evaporation rate. Of course, the nature of the resin being used is another factor that can affect the final solvent blend choice.

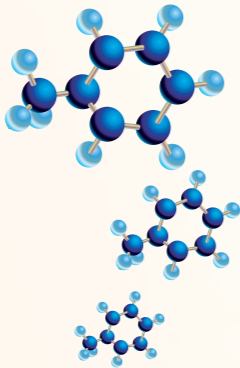
If one substitute Toluene by Acetone for instance, several issues such as hardening during calendaring operations, dry tack development, demixing, etc... may be encountered as Acetone has a very different volatility and solvency power than Toluene.

On the other hand, a solvent such as MethylCyclohexane - which is closer in behavior to Toluene – allows reaching the reference formulation characteristics more easily, and thus reduces the chances of encountering these problems.

Examples of possible substitution blends for a reference containing 60 w % Toluene are displayed in Table VI.

Table VI

Compound wt %	Reference	Blend 1	Blend 2	Blend 3
Solane 60/95				45
Acétate d'éthyle	30	35	25	25
Methyl cyclo-hexane		35	50	
Methyl Ethyl Ketone	10	30	25	30
Toluene	60			
Densité	0.865	0.818	0.8305	0.752
Hansen Solubility Parameters (sqrt/ J/cm³)				
δ <sub>D</sub>	3.35	4.46	3.46	3.65
δ <sub>H</sub>	3.84	3.91	2.96	2.95
δ <sub>P</sub>	17.15	15.94	15.95	15.50
δ total	17.89	17.00	16.59	16.20



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Alternatives  
to Toluene & Xylene:  
TOTAL's answer for industry



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# Alternatives to Toluene & Xylene:

Toluene and Xylene are used as thinners or solvents in a variety of industries including paints & coatings, resins, inks, adhesives, industrial cleaners, ...

The European Union has recently introduced a number of new directives and proposals that have an important impact upon the use of both Toluene & Xylene in your applications. This brochure has been designed to clarify these changes, and also explain which products TOTAL Special Fluids proposes as replacements.

If you do not find the products you are looking for listed in this brochure, all is not lost, as TOTAL Special

Fluids offers an extensive range of over 120 specialty hydrocarbon fluids that have been developed in partnership with our customers. This process can begin with a simple phone call, why not pick up the phone today and we can get started ?

## What legislation should I be aware of? What does this mean for my products?

### TOLUENE (CAS No 108-88-3)

#### European Directive 67/548/EC

- The TOLUENE classification and labelling requirements have been updated: Toluene is recognised as Toxic to Reproduction Category 3. Member States are required to comply with this directive by **31 October 2005**.
- If the Toluene threshold value of **≥ 5% by mass** is exceeded, then the formulation must be labelled with the risk phrase relevant to Toluene.

#### European Directive 2005/59/EC

- Toluene may not be placed on the market or used as a substance or constituent of preparations in a concentration equal to or higher than 0,1% by mass in **adhesives and spray paints intended for sale to the general public**.
- These measures shall be applied from 15 June 2007.

### XYLENE (CAS No 1330-20-7)

#### Pending new classification of Ethyl Benzene (CAS No 100-41-4)

- Regulation with regard to the classification for Ethyl Benzene is important for us as standard mixed Xylene can include up to 20% Ethyl Benzene.
- Discussion is at present ongoing within the European bodies that may result in an update to the classification and labeling of fluids containing Ethyl Benzene.

### CYCLOHEXANE (CAS No 110-82-7) Einecs No: 203-806-2

#### European Directive 1348/2008/EC

- Shall not be placed on the market for the first time after 27 June 2010, for supply to the general public, as a constituent of neoprene-based contact adhesives in concentrations equal to or greater than 0,1 % by mass in package sizes greater than 350 g.
- Neoprene-based contact adhesives containing cyclohexane and not conforming to paragraph 1 shall not be placed on the market for supply to the general public after 27 December 2010.
- Without prejudice to other Community legislation concerning the classification, packaging and labelling of dangerous substances and preparations, neoprene based contact adhesives containing cyclohexane in concentrations equal to or greater than 0,1 % by mass that are placed on the market for supply to the general public after 27 December 2010 shall be visibly, legibly and indelibly marked as follows:
  - This product is not to be used under conditions of poor ventilation.
  - This product is not to be used for carpet laying."

# Which alternative products can be used ?

TOTAL Special Fluids has developed a series of hydrocarbon fluids that display both the technical characteristics and application behavior you require as a user of Toluene or Xylene.

In your application, the replacement of Toluene and Xylene is driven by required technical characteristics such as solvency power, evaporation rate and/or health and safety concerns. Total Special Fluids has a wide range of Aromatic products, "Cycloparaffinic" and "Paraffinic" fluids to answer your needs.

In the Table below some examples of alternate solvents are described. Both Cycloparaffinic and Paraffinic fluids serve as effective replacements to Toluene or Xylene. Lighter products are suitable alternative for Toluene, whereas heavier products are often used for Xylene substitution.

Table I : Cycloparaffinic solvents

Characteristics	Unit	Méthod	Cyclohexane	Methyl Cyclohexane	TOLUENE
Density at 15°C	kg/m³	ASTM D4052	783	774	871
Boiling range	°C	ASTM D86	81-82	100-103	109-111
Flash Point PM	°C	ISO 3679	<-20	0	4
Viscosity at 20°C	mm²/s	ASTM D445	1.25	0.95	0.70
Evaporation rate	Ether=1	DIN 53170	2	14	6
Aniline point	°C	ASTM D611	31	40	9 (mixed)

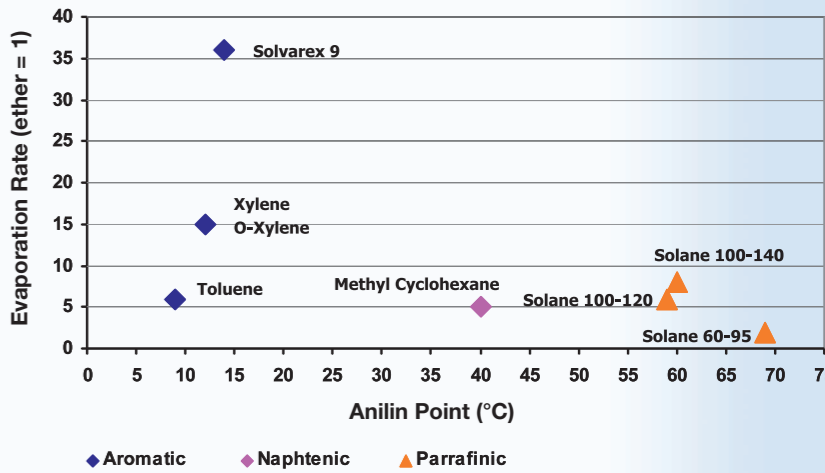
Table II : Paraffinic solvents

Characteristics	Unit	Méthod	Solane 60/95	Solane 80/110	Solane 100/120	Solane 100/140
Density at 15°C	kg/m³	ASTM D4052	680	695	728	730
Boiling range	°C	ASTM D86	62-95	83-108	102-123	103-135
Flash Point PM	°C	ISO 3679	-26	-12	2	4
Viscosity at 20°C	mm²/s	ASTM D445	0.5	0.7	0.7	0.7
Evaporation rate	Ether=1	DIN 53170	2	3.2	6	8
Aniline point	°C	ASTM D611	69	68	59	60

Tableau III : Aromatic solvents

Propriété	Unité	Méthode	Solvarex 9	Solvarex 10	O-Xylene	Xylene
Density at 15°C	kg/m³	ASTM D4052	875	890	884	870
Boiling range	°C	ASTM D850	160-175	188-215	144-145	137-143
Flash Point PM	°C	ASTM D93		68		
		ISO 13736	43		30	26
Evaporation rate	Ether=1	DIN 53170	36	130	14	15
Aniline point	°C	ASTM D611	14	16	ND	12

To help you in your choice, the graph below illustrates the evaporation rate / aniline point relationship for some of the products.



## XYLENE

For some applications, these solvents can be used as a direct replacement. When a direct replacement is not possible, there is a need to use a solvent blend instead, thus often requiring reformulations.

When looking for Xylene replacement the most direct alternative is O-Xylene which displays the same characteristic, especially solvency power and evaporation rate. The other direct alternative is the aromatic cut SOLVAREX 9 or 10, which display an excellent solvency power, but higher evaporation rate. These products are free of Ethyl benzene and are very effective alternatives, especially for coil coatings, baked coatings, alkyd resin synthesis, etc...

Xylene can be effectively replaced by Solvarex 9 in alkyd resin synthesis. In addition - thanks to its higher flash point - presence of residual Solvarex solvent will have little or no effect on the final flash point after the dilution step with white spirits.

In industrial paint formulation, Solvarex 10 will prove to be an effective replacement for Xylene. Its low evaporation rate as well as its high flash point will allow for a better evaporation profile adjustment. This will enable the formulator to achieve formulations compliant with current requirements in terms of VOCs (< 420 g/L) and viscosity (< 30 s coupe AFNOR 4).

When a blend is required, various blend solutions are available. The best option will be retained based on the targeted final evaporation rate, flash point and Hansen solubility parameters. For example, as shown in Table IV, Blends 1, 2 or 3 can be potential substitutes for an 80/20 Xylene/BuAc formulation.

Table IV

Compound wt %	Reference	Blend 1	Blend 2	Blend 3
Methyl cyclohexane		70	40	50
Solane 60/95			30	
MEK				30
N-butyl acetate	20	30	30	20
Xylene	80			
Density g/L	0.860	0.798	0.762	0.799
Hansen Solubility Parameters (sqrt/ J/cm³)				
δ <sub>p</sub>	1.53	1.01	0.97	3.37
δ <sub>H</sub>	3.73	1.80	1.68	2.73
δ <sub>D</sub>	17.25	15.95	15.64	15.96
δ total	17.71	16.08	15.76	16.54